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Multiscale Structural Model of Super Carbon Nanotubes

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Abstract

Extraordinary mechanical properties in biological composites come from their hierarchical structures and are well seen in bones, teeth, shells etc. Nature inspired knowledge could certainly help in the design of new nanostructured materials. The current study illustrates a multi-scale nanotube model for the purpose of the structure of very large groups of carbon nanotubes (CNTs). Two different types of circular beam finite elements are used to shape bond stretching energy or to account for the potential connected to bond angle variation. Multiscale approach considers CNTs at a mesoscopic level through chains of straight cylindrical segments, where mesoscopic force field describes the interactions among the segment. Property dependence at the nanoscale results from the surface and bulk energies competition.

Keywords: Hierarchy; Super Carbon Nanotube; Numerical Model

1 Introduction

For a material to have superior mechanical properties the limits of improving one property by sacrificing another should be overcome. Hierarchical structures of exceptional properties are widespread in biosystems such as bones, teeth, shells, collagen tissues etc. The knowledge on hierarchical biomaterials could obviously help design new nanostructured technical materials and products. Thus, scientists are suggesting materials property control at multiscale levels. Mathematical models involved in hierarchical materials design reported consider: self-similar and multiple reinforced composites, bio-inspired structures, ceramic based nanocomposites and fibre reinforced composites. The methods used are based on global-local finite element, domain decomposition and superposition techniques [1-3].

The fourth allotrope of condensed carbon is carbon nanotube. Carbon nanotubes are rolled-up cylinders of graphene sheets with tubule diameters sometimes small to have 1D periodicity. Plenty of attention is paid to carbon nanotubes (CNTs) because of their special structural and transport features, including excellent tensile strength, high modulus, good electrical and thermal conductivity and low density [4-6]. Significant mechanical and physical properties of individual

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carbon nanotubes encourage researchers to develop continuous high performance fibres and ropes based on carbon nonotubes. Some studies reported on the molecular mechanics modelling of the pull-out force between adjacent CNTs in double wall carbon nanotubes [7], others focused on super-nanotubes super-graphene and super-square systems continuum modelling, with the use of equivalent beam concept [8]. Nanostructures with an optimal distribution of nanoelements (nanoclay, carbon nanotubes, nanoparticles and nanofibres) enable a great increase in properties and functionality [9]. Some microstructure recipes such as multilayer configuration, hierarchical tree structures, bundle and yarns can be considered as elements of the bio-inspired design of industrial materials.

A number of carbon nanotubes have been assembled by hierarchical super carbon nanotubes (SCNT). Lowest order (SCNT) is the building block of the second one, and the latter for the next one and so on, Fig. 1. Thus a kind of hierarchical structure can be obtained with exceptional properties, not existing in original structures previously [1, 10].

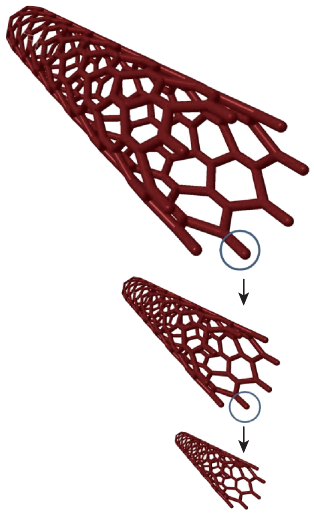

Fig. 1: The hierarchical CNT super structure

Macro-scale super carbon tubes were investigated because of self-similarity breakage [11]. In this study an example of the super CNTs numerical nanostructure modelling is carried.

2 Numerical Model-carbon Nanotubes Super Structures

Materials are modelled using phenomenological/continuum models or force constant, bond angle bending force constant and torsion resistance respectively and quantum/molecular mechanics models. However, the material length and time scales for the molecular mechanics model simulations are still limited by the available computational power, and such methods are prohibitive in the analysis of nanoscale devices. It is therefore important to extend the multiscale mechanics concepts as an efficient tool to analyse the mechanical response of nanoscale structures. For the analysis of complex nanostructures geometries and boundary conditions encountered in nanotechnology applications, a versatile numerical model such as the coarse-grain method, quasi-continuum method, concurrent and hierarchical multiscale method was developed.